



Symbolic Computational Approach to the Marangoni Convection Problem With Soret Diffusion

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SYMBOLIC COMPUTATIONAL APPROACH TO THE MARANGONI CONVECTION PROBLEM WITH SORÉT DIFFUSION

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ABSTRACT

A recently reported solution for stationary stability of a thermo-solutal system with Sorét diffusion is re-derived and examined using a symbolic computational package. Symbolic computational languages are well suited for such an analysis and facilitate a pragmatic approach that is adaptable to similar problems. Linearization of the equations, normal mode analysis, and extraction of the final solution are performed in a *Mathematica*[®] notebook format. An exact solution is obtained for stationary stability in the limit of zero gravity. A closed form expression is also obtained for the location of asymptotes in relevant parameter, (Sm_c, Ma_c) , space. The stationary stability behavior is conveniently examined within the symbolic language environment. An abbreviated version of the *Mathematica*[®] notebook is given in the Appendix.[†]

NOMENCLATURE

C	concentration
c	disturbance concentration
$D_{m,n}$	diffusivity elements surface tension
D_m	Dufour coefficient, $\frac{D_{12} \gamma_1}{D_{11} \gamma_2}$
d	depth of fluid layer
h	surface heat transfer coefficient
h_s	surface mass transfer coefficient
J	mass flux from surface
Ma	Marangoni number, $\frac{\gamma_1 d \Delta T}{D_{11} \mu}$
Nu	surface Nusselt number, $\frac{hd}{\rho c_p D_{11}}$
Pr	Prandtl number, ν/D_{11}
ΔP	pressure difference
Δp	disturbance pressure difference
Q	heat flux from surface

Sh	surface Sherwood number, $\frac{h_s d}{D_{22}}$
Sm	Sorét coefficient, $\frac{D_{21} \gamma_2}{D_{22} \gamma_1}$
T	temperature
t	time
\bar{U}	velocity vector
U	x-component velocity
\bar{u}	disturbance velocity vector
V	y-component velocity
W	z-component velocity
w	z-component disturbance velocity
x,y,z	Cartesian coordinates (see Fig. 1)

Greek Symbols

α	wavenumber
γ	surface tension variation
θ	disturbance temperature
ϕ	normal mode temperature
λ	eigenvalue
μ	dynamic viscosity
ν	kinematic viscosity
ρ	density
σ	surface tension
τ	diffusivity ratio, D_{22}/D_{11}
χ	normal mode concentration

Subscripts

0	value at $z = 0$
1	value at $z = 1$
b	basic state
c	critical value
∞	asymptotic value

[†]The unabridged *Mathematica*[®] notebook is available from the author or on the internet at <http://zeta.lerc.nasa.gov/6712/people/skarda.htm>

INTRODUCTION

This paper is intended to achieve three goals. First the paper and an associated *Mathematica*[®] notebook document the derivation details of an exact solution for stationary stability of the Marangoni-Benard system with Soret diffusion (Skarda et. al., 1998). Second, it is hoped that the problem described herein might serve as a “hands on learning tool” to augment teaching or understanding of linear stability. The individual steps of a linear stability analysis and their relationship to each other can effectively be examined within a symbolic computational environment. Finally, several features of symbolic computational languages such as *Mathematica*[®] (Wolfram, 1996), are demonstrated within the notebook that can greatly benefit similar analyses. In fact, various elements of the notebook are directly, or with minor modification, applicable to a wide range of stability problems. For example the brief linearization function we construct is quite general and can be applied to linearize systems of nonlinear partial differential equations (p.d.e.) of arbitrary order and degree, as well as the associated boundary conditions. Similarly, the normal mode substitutions apply to most autonomous systems, where the boundary conditions can also be satisfied by the normal mode solutions.

The physical problem under consideration is that of binary fluid convection with soret diffusion. Hurle and Jakeman (1969 and 1971) showed that these binary systems can be quite sensitive to the Soret effect resulting in either undesirable flows due to trace amounts of impurities or desirable mixing by providing a small concentration of solute. Binary fluid systems are also instructive because they can be represented as relatively simple fluid-dynamical systems with constant coefficients (Jacqmin, 1996) and zero base flow. The convection displays an abundance of interesting phenomena as demonstrated by several theoretical and experimental investigations, e.g., Kolodner et. al. (1989), Bensimon et. al. (1990), Glazier and Kolodner (1991), Cross (1986), Knobloch and Moore (1988). In these studies, flow is driven due to density variations. More recent investigations have examined the Soret effect in systems where surface tension gradients at the free surface drive flow (Chen and Chen 1994, Castillo and Velarde, 1978, and Bergeon, et. al., 1994, Skarda, et. al., 1998). Such phenomena is important to proposed containerless processing applications in microgravity.

We discuss the linear instability of double diffusive convection with the Soret effect that is driven by surface tension variation along the free surface. An imposed temperature difference across the layer, ΔT_b , induces a concentration difference, ΔC_b . We rescale the problem in the absence of buoyancy which leads to a concise representation of neutral stability results in and near the limit of zero gravity. An exact solution is obtained for stationary stability. One important consequence of the exact solution is the validation of published numerical results in the limit of zero gravity. Moreover, the precise location of asymptotes in relevant parameter, (Sm_c, Ma_c) , space are computed from exact solutions. Stability behavior is briefly examined using the exact solution. The process of linearizing the equations, deriving the normal mode equations, and obtaining an exact solution for neutral stability are illustrated in the Appendix in *Mathematica*[®] notebook format.

DEVELOPMENT OF EQUATIONS

We consider the unbounded cross-doubly diffusive fluid layer of depth d as shown in Fig. 1. Buoyancy is neglected, and onset of con-

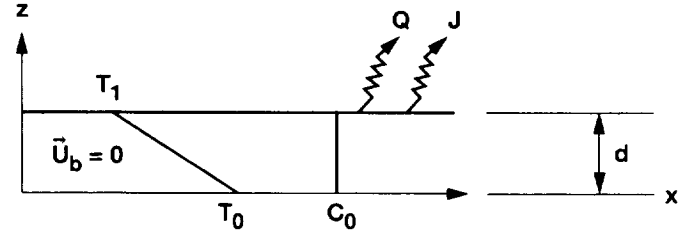


Figure 1.—Unbounded double diffusive fluid layer.

vection due to surface tension variation is examined. The basic or unperturbed state is one of no flow, $U_b = 0$, an imposed temperature profile across the layer, $T_b(z) = T_b(0) - \Delta T_b \frac{z}{d}$, and an induced concentration gradient across the layer, $\Delta C_b = -\frac{D_{21}}{D_{22}} \Delta T_b$. Difference quantities of the form, Δy_b , are defined as $\Delta y_b = y_b(0) - y_b(d)$.

The governing equations we wish to linearize are:

$$\bar{\nabla} \cdot \mathbf{U} = 0 \quad (1)$$

$$\rho \frac{D\bar{\mathbf{U}}}{Dt} = -\bar{\nabla}P + \mu \bar{\nabla}^2 \bar{\mathbf{U}} \quad (2)$$

$$\frac{DT}{Dt} = D_{11} \bar{\nabla}^2 T + D_{12} \bar{\nabla}^2 C \quad (3)$$

$$\frac{DC}{Dt} = D_{21} \bar{\nabla}^2 T + D_{22} \bar{\nabla}^2 C \quad (4)$$

The dynamic viscosity, μ , and diffusivity elements, D_{mn} , are assumed constants. The boundary conditions are:

$$\text{At } z=0, \bar{\mathbf{U}}(0)=0, \left(\frac{\partial U_x}{\partial x}, \frac{\partial U_y}{\partial y}, \frac{\partial U_z}{\partial z} \right) = 0, T(0) = T_0, C(0) = C_0 \quad (5a \text{ to } 5d)$$

$$\begin{aligned} \text{At } z=d, \bar{\mathbf{U}}(0)=0, \mu \left[\left(\frac{\partial U_z}{\partial x} + \frac{\partial U_x}{\partial z} \right) \hat{i} + \left(\frac{\partial U_z}{\partial y} + \frac{\partial U_y}{\partial z} \right) \hat{j} \right] \\ = -\gamma_1 \bar{\nabla}_{\parallel} T - \gamma_2 \bar{\nabla}_{\parallel} C \quad (6a \text{ to } 6c) \end{aligned}$$

where $\nabla_{\parallel} = \hat{i} \frac{\partial}{\partial x} + \hat{j} \frac{\partial}{\partial y}$. Surface tension, σ , is approximated as a linearized function of T and C , $\sigma = \sigma_0 - \gamma_1(T - T_b) - \gamma_2(C - C_b)$, where γ_1 and γ_2 are the temperature and concentration variations with surface tension, $\gamma_1 = -\left(\frac{\partial \sigma}{\partial T} \right)_{C,P}$ and $\gamma_2 = -\left(\frac{\partial \sigma}{\partial C} \right)_{T,P}$. Heat and mass flux conditions are

$$\rho c_p \left(-D_{11} \frac{\partial T}{\partial z} - D_{12} \frac{\partial C}{\partial z} \right) = Q \quad (6d)$$

$$-D_{21} \frac{\partial T}{\partial z} - D_{22} \frac{\partial C}{\partial z} = J \quad (6e)$$

where the density, ρ , and specific heat, c_p , are constants. The surface heat and mass fluxes, Q and J are expanded as:

$$Q = Q(T_b, C_b) + \left. \frac{\partial Q}{\partial T} \right|_{T_1} (T(1) - T_1) \quad (7a)$$

$$J = J(T_b, C_b) + \left. \frac{\partial J}{\partial C} \right|_{C_1} (C(1) - C_1) \quad (7b)$$

Substituting Eq. (7a) into Eq. (6d), and Eq. (7b) into Eq. (6e) for Q and J , respectively, facilitates linearization of the flux conditions.

The dependent variables are written in terms of the base flow and perturbation variables, $\bar{U} = \bar{u}$, $T = T_b + \theta$, $C = C_b + c$, and $\Delta P = \Delta P_b + \Delta p$. Substituting these into the governing equations and boundary conditions, and retaining only the first order terms leads to the linearized system. Exploiting the pattern matching and limit evaluation capabilities of *Mathematica*[®], a succinct function was constructed to linearize a nonlinear p.d.e of arbitrary order and degree. This linearization function, *Linearize* [equation], is given in the Appendix. Our problem was easily linearized, symbolically, as is illustrated within the notebook in the Appendix.

As is common practice (Chandrasekhar, 1981) the curl operator is applied twice to the momentum equation. This operation could also be performed using the *Mathematica*[®] vector calculus operators.

Following the classical treatment for the Benard type problems, the linearized equations are now nondimensionalized (Chandrasekhar, 1981). Here, they are nondimensionalized using the reference values of Skarda et. al. (1998) for length, velocity, time, temperature, and concentration which are defined as

$$d, \frac{D_{11}}{d}, \frac{d^2}{D_{11}}, \Delta T_b, \text{ and } -\frac{D_{21}}{D_{22}} \Delta T_b.$$

The resulting nondimensional parameters are the Prandtl number, Pr , diffusivity ratio, τ , Dufour coefficient, Dm , Soret coefficient, Sm , Marangoni number, Ma , surface Nusselt Number, Nu , and surface Sherwood number, Sh as defined in the nomenclature. The complete set of dimensionless disturbance equations are given by Eqs. (A.4) to (A.8d) in the Appendix.

A normal mode analysis is performed by assuming solutions of the form $(u, \theta, c) = (w(z), \phi(z), \chi(z))e^{\lambda t + i(\alpha_x x + \alpha_y y)}$. In *Mathematica*[®] this is conveniently done by defining the solutions as the functions, Eqs. (A.9a) to (A.9c) in the Appendix.

These solutions are substituted into the set of linearized Eqs. (A.4) to (A.8d) leading to a 4th order and two 2nd order ODE's. The normal mode equations are easily obtained by evaluating the *Mathematica*[®]

cells for the linearized equations **after** evaluating the solution forms, Eqs. (A.9a) to (A.9c). The resulting normal mode equations are also given in (Skarda et. al., 1998). The energy and species equations are coupled by their cross diffusive terms which also occur in the flux boundary conditions at $z = 1$. The momentum equation is coupled with both energy and species equations through the tangential stress condition, Eq. (A.8b).

The eigenvalue, λ in Eqs. (9a) to (c) is complex. If the real part of λ is positive, a disturbance in the system grows, and if the real part is negative, the disturbance decays. If $\lambda = 0$, the disturbance persists unchanged in time and the system is in a state of neutral stability. By setting $\lambda = 0$, we can decouple the energy and species equations and directly solve the following normal mode equations for stationary stability.

$$0 = Pr(D^2 - \alpha^2)^2 w \quad (8)$$

$$(D^2 - \alpha^2)\phi = d_\phi Ma \quad w \quad (9)$$

$$(D^2 - \alpha^2)\chi = d_\chi Ma \quad w \quad (10)$$

where

$$d_\phi = \frac{\tau + SmDm}{\tau - \tau SmDm} \quad \text{and} \quad d_\chi = \frac{1 + \tau}{\tau - \tau SmDm}$$

The corresponding normal mode boundary conditions are given below:

At the lower surface, $z = 0$,

$$w(0) = 0 \quad (11a)$$

$$Dw(0) = 0 \quad (11b)$$

$$\phi(0) = 0 \quad (11c)$$

$$\chi(0) = 0 \quad (11c)$$

At the upper surface, $z = 1$,

$$w = 0 \quad (12a)$$

$$-D^2 w = \alpha^2 (\phi - Sm\chi) \quad (12b)$$

$$D\phi - Sm Dm D\chi + Nu \phi = 0 \quad (12c)$$

$$-D\phi + D\chi + Sh \chi = 0 \quad (12d)$$

STATIONARY SOLUTION

The solution forms of w , ϕ , and χ are easily determined from inspection of Eqs. (8) to (10) and are given in the Appendix by Eqs. (A.12) to (A.14). Determination of the integration constants for this problem is tedious. Evaluation of b_1 and c_1 from Eqs. (A.21) and (A.22) should confirm this claim. A highly desirable feature of symbolic languages is their ability to minimize much of the computational drudgery, verify results obtained by other means, and often simplify the final expression to a tractable form. The use of *Mathematica*[®] to solve for integration coefficients, b_1 and c_1 , certainly minimizes drudgery, and we will find below that the final form of the neutral stability solution is simplified by *Mathematica*[®] to a tractable form. An expression for neutral stability is obtained by applying the tangential stress balance, Eq. (12b). This yields the following exact solution, Eq. (13), for stationary stability of the double diffusive Soret problem (Skarda et. al., 1998). For general-ity the Dufour diffusivity term is also retained in the energy equation.

$$\frac{\text{Ma} \left\{ \left(\text{Sm} \left(1 + \frac{1 - \text{Dm}}{\tau} \right) - 1 \right) \alpha \cosh \alpha + \left(\frac{\text{Nu}}{\tau} \text{Sm} - \text{Sh} \right) \sinh \alpha \right\}}{2 \left\{ (\text{Sm} \text{Dm} - 1) \alpha^2 (1 + \cosh 2\alpha) + \text{Nu} \text{Sh} (1 - \cosh 2\alpha) - (\text{Nu} + \text{Sh}) \alpha \sinh 2\alpha \right\}} + \frac{8\alpha^2 - 4\alpha \sinh 2\alpha}{\sinh 3\alpha - 3\sinh \alpha - 4\alpha^3 \cosh \alpha} = 0 \quad (13)$$

RESULTS

The neutral stability curves shown in Figs. 2 and 3 are computed directly from Eq. (13). The abscissa and ordinate are the wavenumber and the Marangoni number, respectively, and the eigenvalue, λ , is zero along each curve. For Ma values above a neutral stability curve (corresponding to given Sm and τ values), infinitesimal disturbances grow in time and the fluid layer is said to be unstable. The layer is linearly stable for Ma values below the appropriate neutral stability curve. In Fig. 2, the curves are shifted upward for increasing values of Sm thus increasing Sm has a "stabilizing effect." In Fig. 3, decreasing τ values are destabilizing, shifting the neutral stability curves downward. We emphasize that these are stationary stability results; however, oscillatory stability will occur before stationary stability (Ma values below the stationary values) for certain ranges of Sm values (Chen and Chen, 1994, Skarda et. al., 1998).

The minimum value of Ma on each curve in Figs. 2 and 3 is called the critical Marangoni number, Ma_c , and is of interest since onset of instability typically occurs at this value. In Fig. 4, stationary stability boundaries, the loci of points consisting of Ma_c values, are shown in $(\text{Sm}_c, \text{Ma}_c)$ space for different values of τ . The overall behavior is quite similar to the Rayleigh-Benard stationary stability results presented in $(\text{Sr}_c, \text{Ra}_c)$ space by Hurle and Jakeman (1971) where the Soret coefficient, Sr , and Rayleigh number, Ra , are defined in the usual manner (Hurle and Jakeman 1971). Asymptotic behavior occurs at a finite Sm_c value and Ma_c is driven to zero as $|\text{Sm}_c| \rightarrow \infty$. The exact location of the asymptote observed in Fig. 4 is also determined from our solution, Eq. (13), and is given in Skarda et. al., (1998). For flux boundary conditions often applied to the Soret problem, $\text{Nu} = \text{Sh} = 0$, and $\text{Dm} = 0$ the location of the asymptote reduces to a simple function of τ , $\text{Sm}_\infty = \left(1 + \frac{1}{\tau} \right)^{-1}$. This result was found to be identical to the asymp-

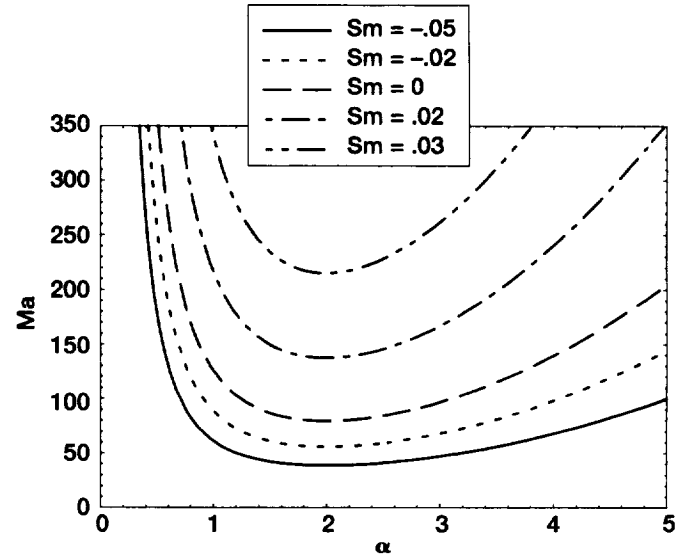


Figure 2.—Neutral stability curves, each curve for constant Sm values, $\tau = .05$, $\text{Dm} = 0$, $\text{Nu} = 0$, $\text{Sh} = 0$.

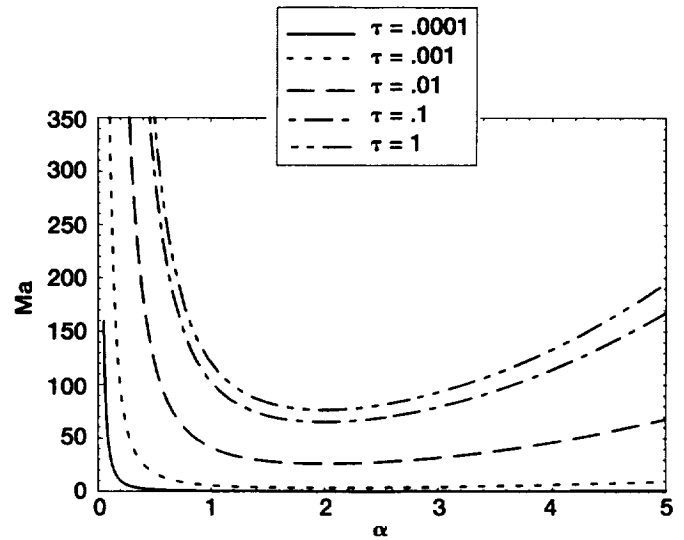


Figure 3.—Neutral stability curves, each curve for constant τ values, $\text{Sm} = -.02$, $\text{Dm} = 0$, $\text{Nu} = 0$, $\text{Sh} = 0$.

tote location expression obtained by Hurle and Jakeman (1971), but in $(\text{Sr}_c, \text{Ra}_c)$ space, for the case of the buoyancy induced Soret problem with free-free surfaces (Skarda et. al. 1998). As before oscillatory instability which must be computed numerically, is not considered in this analysis, but is discussed in the previously mentioned references.

CONCLUSIONS

The exact solution for stationary onset of convection for Marangoni-Benard instability with Soret effect was successfully

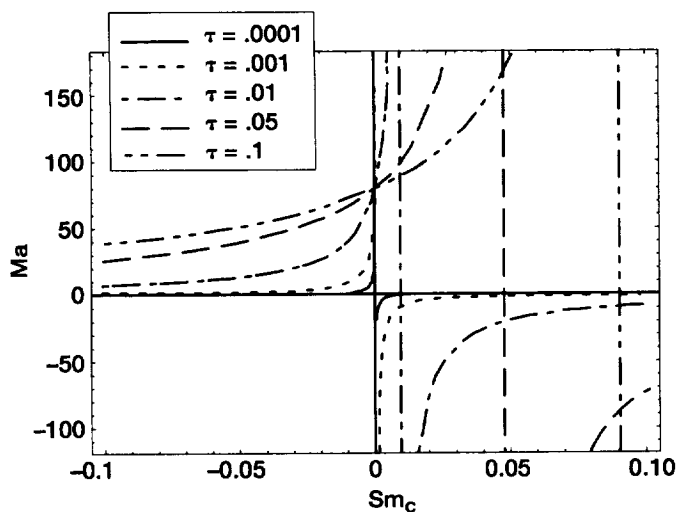


Figure 4.—Stationary stability boundaries, each curve for constant τ values, $\alpha_c = 1.99$, $Dm = 0$, $Nu = 0$, $Sh = 0$.

derived using a symbolic computational package, *Mathematica*®. The results agree with the “hand-derived” form of the solution recently reported in the literature. The associated notebook permits users to reconstruct the steps leading to the solution. The exact solution is also provided in a form to allow immediate examination of neutral stability behavior and exploration of various parametric effects. While exact solutions are uncommon, various parts of the notebook can be applied with little modification to assist with aspects of other linear stability problems.

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APPENDIX

Exact Solution For Stationary Stability Double Diffusive Marangoni Problem With Soret Diffusion

Cross-Diffusion Terms Are Included in Governing Equations & in the Flux BC's at $z=1$
A Conductive/Permeable Base Is Considered at $z=0$

```
<<Calculus'VectorAnalysis';
SetCoordinates[ Cartesian[x,y,z] ];

(* Define linearization function *)
Linearize[equation_] := Limit[Expand[(Expand[equation] /.  $\epsilon^n \rightarrow 0$ ) /  $\epsilon$ ],  $\epsilon \rightarrow \text{Infinity}$ ]
```

■ Governing Equations – Momentum, Energy, Species

```
UMomEq = (* A.1 *)

$$\partial_t U[x, y, z, t] + \{U[x, y, z, t], V[x, y, z, t], W[x, y, z, t]\} \cdot \text{Grad}[U[x, y, z, t]] - \partial_x P[x, y, z, t] + \text{Laplacian}[U[x, y, z, t]];$$


EnergyEq = (* A.2 *)

$$\partial_t T[x, y, z, t] + \{U[x, y, z, t], V[x, y, z, t], W[x, y, z, t]\} \cdot \text{Grad}[T[x, y, z, t]] - D_{11} \text{Laplacian}[T[x, y, z, t]] - D_{12} \text{Laplacian}[S[x, y, z, t]];$$


SpeciesEq = (* A.3 *)

$$\partial_t S[x, y, z, t] + \{U[x, y, z, t], V[x, y, z, t], W[x, y, z, t]\} \cdot \text{Grad}[S[x, y, z, t]] - D_{21} \text{Laplacian}[T[x, y, z, t]] - D_{22} \text{Laplacian}[S[x, y, z, t]];$$


U[x_, y_, z_, t_] := 0 +  $\epsilon$  u[x, y, z, t];
V[x_, y_, z_, t_] := 0 +  $\epsilon$  v[x, y, z, t];
W[x_, y_, z_, t_] := 0 +  $\epsilon$  w[x, y, z, t];
P[x_, y_, z_, t_] := 0 +  $\epsilon$  p[x, y, z, t];
T[x_, y_, z_, t_] :=  $T_b[x, y, z, t] + \epsilon \theta[x, y, z, t]$ ;
S[x_, y_, z_, t_] :=  $S_b[x, y, z, t] + \epsilon \chi[x, y, z, t]$ ;

Linearize[UMomEq];
Linearize[EnergyEq];
Linearize[SpeciesEq];
```

■ Linearized Disturbance Equations

```
MDisturbEq =  $\partial_t \text{Laplacian}[u[x, y, z, t]] - \text{Pr Bi harmonic}[u[x, y, z, t]]$  (* A.4 *)

EDisturbEq =  $\partial_t \theta[x, y, z, t] - \text{Laplacian}[\theta[x, y, z, t]] + S_m D_m \text{Laplacian}[c[x, y, z, t]] - M_a u[x, y, z, t]$  (* A.5 *)

SDisturbEq =  $\partial_t c[x, y, z, t] + \tau \text{Laplacian}[\theta[x, y, z, t]] - \tau \text{Laplacian}[c[x, y, z, t]] - M_a u[x, y, z, t]$  (* A.6 *)
```

■ Boundary Conditions

■ at $z=0$

```
u[x, y, 0, t];
 $\partial_{x,z} u[x, y, 0, t];$  (* A.7,a,b,c,d *)
 $\theta[x, y, 0, t];$ 
 $c[x, y, 0, t];$ 
```


■ at $z=1$

$$\begin{aligned} u[x, y, 1, t]; \\ \partial_{z,z} u[x, y, 1, t] + \partial_{x,x} u[x, y, 1, t] + \partial_{y,y} u[x, y, 1, t]; \\ \partial_z \theta[x, y, 1, t] + Dm \partial_z c[x, y, 1, t] + Nu \theta[x, y, 1, t]; \\ Sm \partial_z \theta[x, y, 1, t] + \tau \partial_z c[x, y, 1, t] + Sh c[x, y, 1, t]; \end{aligned} \quad (* A.8 \ a,b,c,d *)$$

■ Assume Normal Mode Solutions of The Form

$$\begin{aligned} u[x_, y_, z_, t_] &:= w[z] \text{Exp}[\lambda t + I (\alpha_x x + \alpha_y y)]; \\ \theta[x_, y_, z_, t_] &:= \phi[z] \text{Exp}[\lambda t + I (\alpha_x x + \alpha_y y)]; \\ c[x_, y_, z_, t_] &:= \chi[z] \text{Exp}[\lambda t + I (\alpha_x x + \alpha_y y)]; \end{aligned} \quad (* A.9 \ a,b,c *)$$

■ Normal Mode Equations

$$\begin{aligned} (D^2 - \alpha^2)^2 w[z] &= 0 & (* A.10 *) \\ (D^2 - \alpha^2) \phi[z] &= -d_\phi Ma w[z] & (* A.11 *) \\ (D^2 - \alpha^2) \chi[z] &= -d_\chi Ma w[z] & (* A.12 *) \end{aligned}$$

$$(* \text{ where } *) \\ d\phi = (\tau + Sm Dm) / (\tau - \tau Sm Dm); \quad d\chi = (1 + \tau) / (\tau - \tau Sm Dm)$$

■ Solutions For velocity, Temperature, and Concentration Are Expressed As:

$$w[x_] := a1 \sinh[\alpha x] + a2 \cosh[\alpha x] + a3 x \sinh[\alpha x] + a4 x \cosh[\alpha x] \quad (* A.13 *)$$

$$\phi[x_] := b1 \sinh[\alpha x] + b2 \cosh[\alpha x] + b3 x \sinh[\alpha x] + b4 x \cosh[\alpha x] + b5 x^2 \sinh[\alpha x] + b6 x^2 \cosh[\alpha x] \quad (* A.14 *)$$

$$\chi[x_] := c1 \sinh[\alpha x] + c2 \cosh[\alpha x] + c3 x \sinh[\alpha x] + c4 x \cosh[\alpha x] + c5 x^2 \sinh[\alpha x] + c6 x^2 \cosh[\alpha x] \quad (* A.15 *)$$

■ Solve for velocity coefficients, a2, a3, and a4 in terms of a1

Boundary Condition, $w[0] = 0$, $w'[0] = 0$, and $w[1] = 0$ Give

$$a2 = 0; \quad a3 = a1 (\alpha (\cosh[\alpha] / \sinh[\alpha]) - 1); \quad a4 = -a1 \alpha; \quad (* A.16a,b,c *)$$

■ Solve for particular temperature & species solutions

Solve for Particular Solution of ϕ (temperature),
ie solve for b3, b4, b5, b6 (also c3, c4, c5, and c6 values)

$$\begin{aligned} D[b3 \ a1 \ z \sinh[\alpha z] + b4 \ a1 \ z \cosh[\alpha z], \{z, 2\}] - \\ \alpha^2 (b3 \ a1 \ z \sinh[\alpha z] + b4 \ a1 \ z \cosh[\alpha z]) + \\ D[b5 \ a1 \ z^2 \sinh[\alpha z] + b6 \ a1 \ z^2 \cosh[\alpha z], \{z, 2\}] - \\ \alpha^2 (b5 \ a1 \ z^2 \sinh[\alpha z] + b6 \ a1 \ z^2 \cosh[\alpha z]) /. a1 \rightarrow 1 /. d\phi \rightarrow 1 \end{aligned} \quad (* A.17 *)$$

Values of b3, b4, b5, b6 (or c3, c4, c5, or c6) Determined by comparison with Cosh, Sinh, etc Terms of ODE le w[z] Terms

$$\begin{aligned} b3 &= a1 \, d\phi \, Ma \, (\alpha \, \text{Coth}[\alpha] - 1) / (4 \, \alpha^2); & b4 &= -3 \, a1 \, d\phi \, Ma / (4 \, \alpha); & (* \text{ A.18a,b } *) \\ b5 &= a1 \, d\phi \, Ma / 4; & b6 &= -a1 \, d\phi \, Ma \, (\alpha \, \text{Coth}[\alpha] - 1) / (4 \, \alpha); & (* \text{ A.18c,d } *) \end{aligned}$$

$$\begin{aligned} c3 &= a1 \, d\chi \, Ma \, (\alpha \, \text{Coth}[\alpha] - 1) / (4 \, \alpha^2); & c4 &= -3 \, a1 \, d\chi \, Ma / (4 \, \alpha); & (* \text{ A.19a,b } *) \\ c5 &= a1 \, d\chi \, Ma / 4; & c6 &= -a1 \, d\chi \, Ma \, (\alpha \, \text{Coth}[\alpha] - 1) / (4 \, \alpha); & (* \text{ A.19c,d } *) \end{aligned}$$

■ Solve For Homogenous Coefficients – Energy & Species Equations

(* Bottom surface, z=0, is conductive and permeable, therefore: *)

$$b2 = 0; \quad c2 = 0; \quad (* \text{ A.20 a,b } *)$$

Now apply the flux conditions at the top, z=1 and solve for b1 and c1

$$\phi_{\text{fluxbc}} = \phi'[1] + \text{Nu} \, \phi[1] + \quad (* \text{ A.21 } *)$$

$$\begin{aligned} & -\text{Sm} \, \text{Dm} \, \chi'[1]; \\ \chi_{\text{fluxbc}} &= -\phi'[1] + \quad (* \text{ A.22 } *) \\ & \chi'[1] + \text{Sh} \, \chi[1]; \end{aligned}$$

Solve For b1 & c1 simultaneously from flux conditons

$$\begin{aligned} b1 &= .; \quad c1 = .; \\ b1c1 &= \text{Flatten}[\\ & \quad \{b1, c1\} /. \text{Solve}[\{\phi_{\text{fluxbc}}==0, \chi_{\text{fluxbc}}==0\}, \{b1, c1\}]]; \\ b1 &= b1c1[[1]]; \quad c1 = b1c1[[2]]; \end{aligned} \quad (* \text{ A.23 } *)$$

■ Substitute w, ϕ , and χ into tangential stress boundary condition and obtain stationary stability solution

(* The remaining coefficient, a1 will cancel out in boundary condition so we'll set it to 1 *)

$$\begin{aligned} \phi1 &= \phi[1] /. a1->1; \chi1 = \chi[1] /. a1->1; \\ d2w1 &= \text{Simplify}[\text{Expand}[w''[1]] /. a1->1]; \end{aligned}$$

Substitute above into Tangential stress condition at z=1

$$t_{\text{stress}} = \alpha^2 \, \phi1 - \text{Sm} \, \alpha^2 \, \chi1 + d2w1; \quad (* \text{ A.24 } *)$$

Resolve ϕ Term of Tangential Stress Equation – Multiply by 4 Sinh[α] to be Consistent With Literature

$$\phi_{\text{coef}} = 4 \, \text{Simplify}[\alpha^2 \, \phi1] \, \text{Sinh}[\alpha]$$

$$\frac{\text{Ma} \, (\alpha \, (\text{Dm} \, \text{Sm} + \tau) \, \text{Cosh}[\alpha] + \text{Sh} \, \tau \, \text{Sinh}[\alpha]) \, (\alpha^3 \, \text{Cosh}[\alpha] - \text{Sinh}[\alpha]^3)}{\tau \, ((-1 + \text{Dm} \, \text{Sm}) \, \alpha^2 \, \text{Cosh}[\alpha]^2 - (\text{Nu} + \text{Sh}) \, \alpha \, \text{Cosh}[\alpha] \, \text{Sinh}[\alpha] - \text{Nu} \, \text{Sh} \, \text{Sinh}[\alpha]^2)} \quad (* \text{ A.25 } *)$$

$$\phi_{\text{Term}} = \phi_{\text{coef}} / \phi_{\text{coef}}[[5]]$$

$$\frac{\text{Ma} \, (\alpha \, (\text{Dm} \, \text{Sm} + \tau) \, \text{Cosh}[\alpha] + \text{Sh} \, \tau \, \text{Sinh}[\alpha])}{\tau \, ((-1 + \text{Dm} \, \text{Sm}) \, \alpha^2 \, \text{Cosh}[\alpha]^2 - (\text{Nu} + \text{Sh}) \, \alpha \, \text{Cosh}[\alpha] \, \text{Sinh}[\alpha] - \text{Nu} \, \text{Sh} \, \text{Sinh}[\alpha]^2)} \quad (* \text{ A.26 } *)$$

Resolve χ Term of Tangential Stress Equation – Multiply by 4 Sinh[α] to be Consistent With Literature

$$\chi_{\text{coef}} = 4 \text{ Simplify}[\alpha^2 \chi_1] \text{ Sinh}[\alpha]$$

$$\frac{\text{Ma} (\alpha (1 + \tau) \text{Cosh}[\alpha] + \text{Nu Sinh}[\alpha]) (\alpha^3 \text{Cosh}[\alpha] - \text{Sinh}[\alpha]^3)}{\tau ((-1 + \text{Dm Sm}) \alpha^2 \text{Cosh}[\alpha]^2 - (\text{Nu} + \text{Sh}) \alpha \text{Cosh}[\alpha] \text{Sinh}[\alpha] - \text{Nu Sh Sinh}[\alpha]^2)} \quad (* \text{ A.27 } *)$$

$$\chi_{\text{Term}} = -\text{Sm } \chi_{\text{coef}} / \chi_{\text{coef}}[[5]]$$

$$- \frac{\text{Ma Sm} (\alpha (1 + \tau) \text{Cosh}[\alpha] + \text{Nu Sinh}[\alpha])}{\tau ((-1 + \text{Dm Sm}) \alpha^2 \text{Cosh}[\alpha]^2 - (\text{Nu} + \text{Sh}) \alpha \text{Cosh}[\alpha] \text{Sinh}[\alpha] - \text{Nu Sh Sinh}[\alpha]^2)} \quad (* \text{ A.28 } *)$$

$$\text{d2wcoef} = \text{Expand}[4 \text{ Sinh}[\alpha] \text{ d2w1 }] / \phi_{\text{coef}}[[5]]$$

$$\frac{8 \alpha^2 - 4 \alpha \text{Sinh}[2 \alpha]}{\alpha^3 \text{Cosh}[\alpha] - \text{Sinh}[\alpha]^3} \quad (* \text{ A.29 } *)$$

- Collect the ϕ and χ Terms into one term containing the solet coefficient Sm. Then with d2wcoef, generate Neutral Stability Solution.

$$\text{NeutralSoln} = \frac{\text{Simplify}[(\text{Numerator}[\phi_{\text{Term}}] + \text{Numerator}[\chi_{\text{Term}}])]}{\text{Denominator}[\phi_{\text{Term}}] + \text{Numerator}[\text{d2wcoef}]/\text{Denominator}[\text{d2wcoef}]} \quad (* \text{ A.30*} *)$$

$$\frac{\text{Ma} (\alpha (\text{Sm} (-1 + \text{Dm} - \tau) + \tau) \text{Cosh}[\alpha] + (-\text{Nu Sm} + \text{Sh } \tau) \text{Sinh}[\alpha])}{\tau ((-1 + \text{Dm Sm}) \alpha^2 \text{Cosh}[\alpha]^2 - (\text{Nu} + \text{Sh}) \alpha \text{Cosh}[\alpha] \text{Sinh}[\alpha] - \text{Nu Sh Sinh}[\alpha]^2)} + \frac{8 \alpha^2 - 4 \alpha \text{Sinh}[2 \alpha]}{\alpha^3 \text{Cosh}[\alpha] - \text{Sinh}[\alpha]^3}$$

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